

Exploratory Research on Simulation of CO₂-Brine-Mineral Interactions

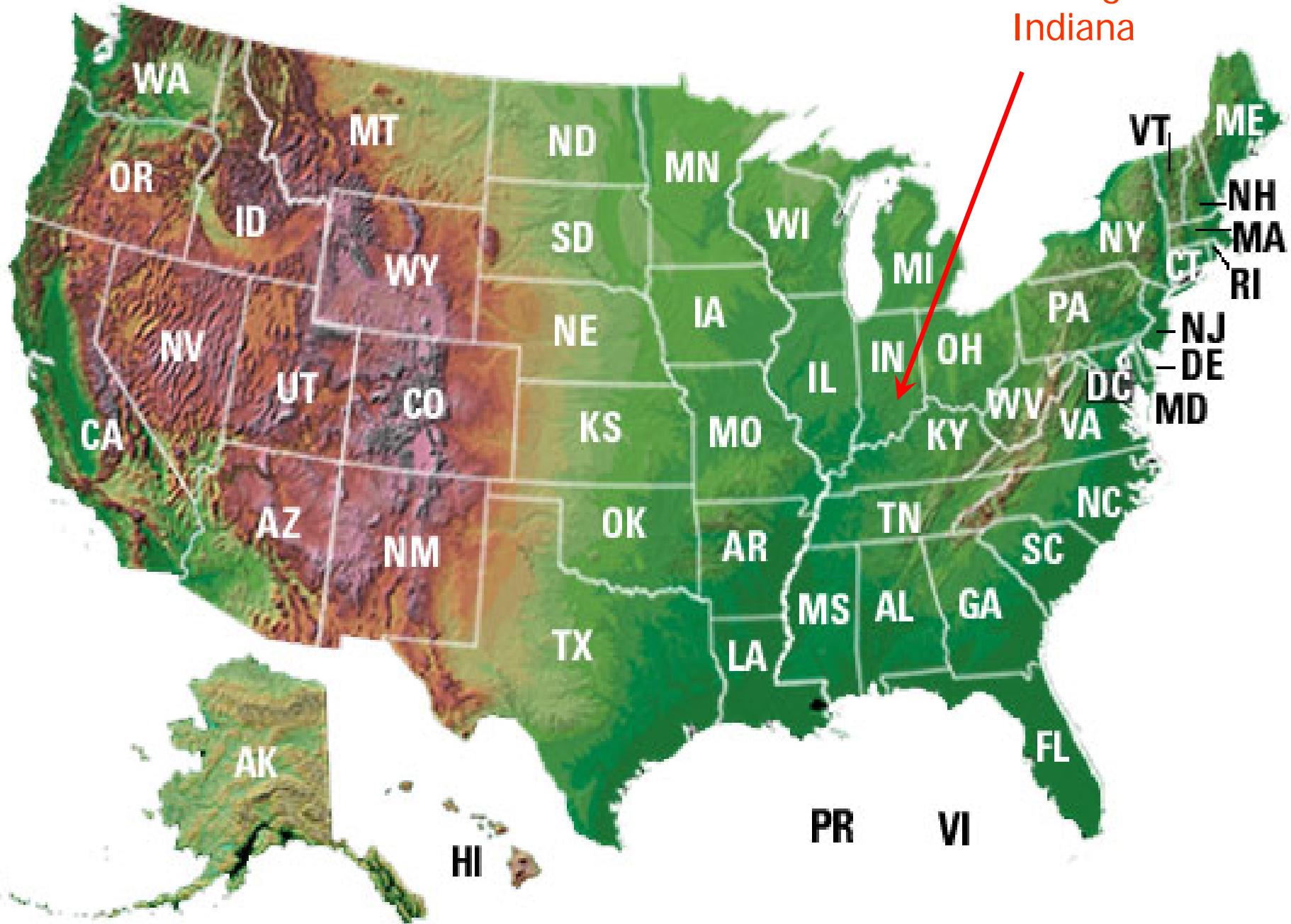
Phase I
Project Manager: David Lang

Substitute Principal Investigator/Project Director:
Shiao-hung Chiang
University of Pittsburgh

Original Principal Investigator
Chen Zhu
Indiana University

Consultant
Zhenhao Duan
University of California – San Diego

Bloomington,
Indiana



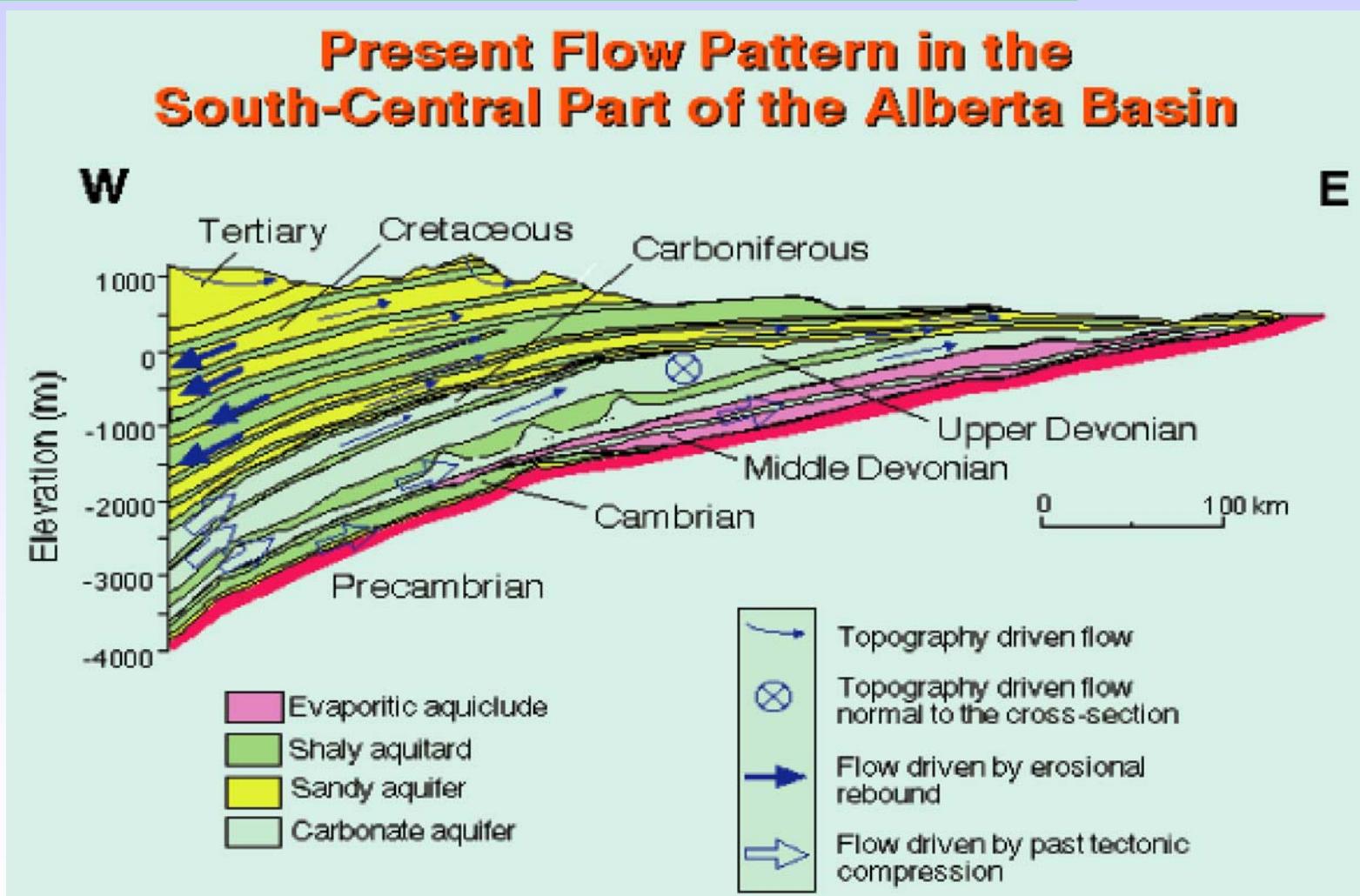


Indiana University
Bloomington, Indiana

CO₂-Brine-Mineral Interactions

- ❖ **For geological sequestration, brine sequestration, mineral sequestration, gas hydrate**
- ❖ **The gas**
- ❖ **The rock**
- ❖ **The brine**
- ❖ **The interactions**

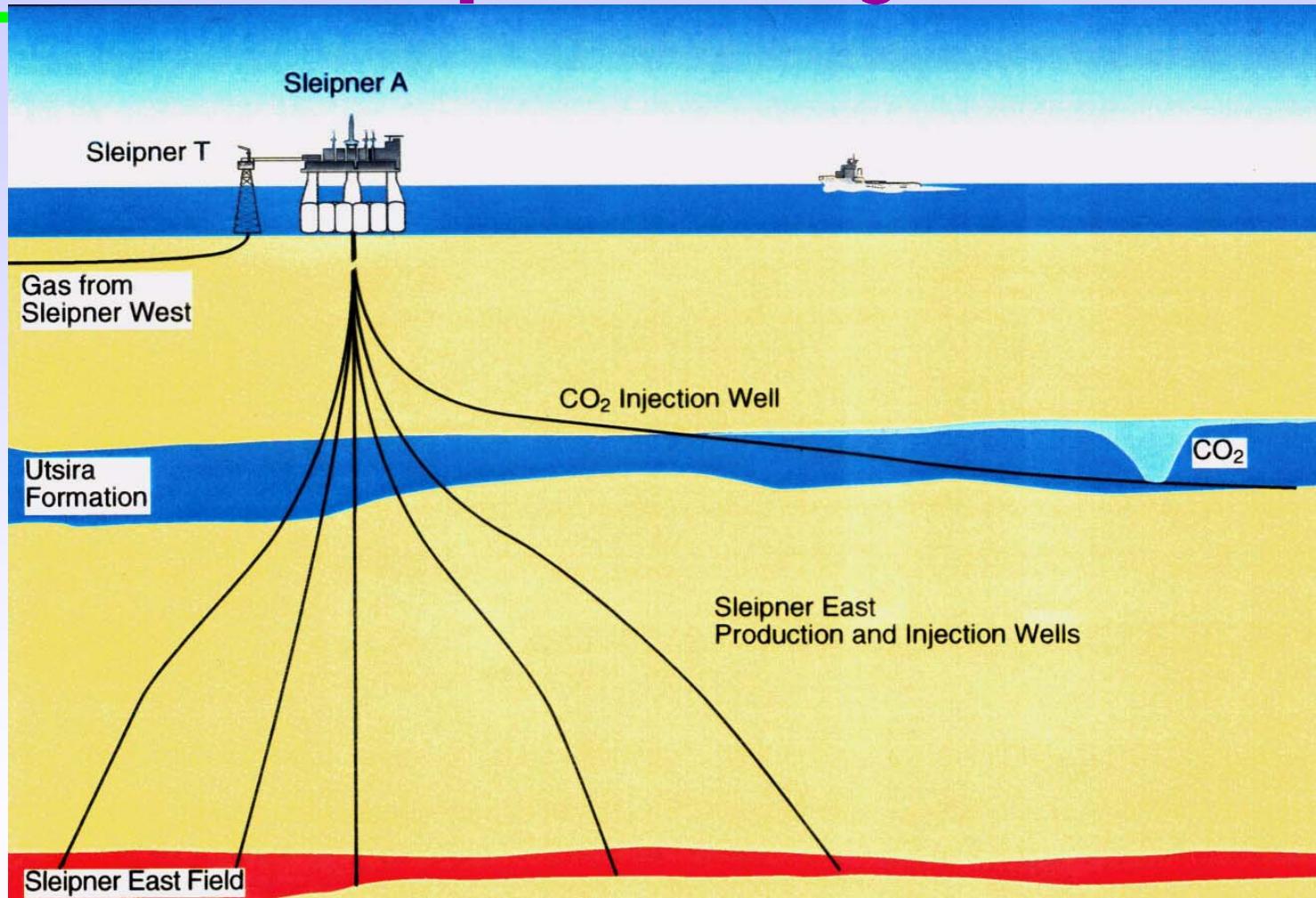
Geological carbon sequestration



From Bill Gunter

BRINEFIELD SEQUESTRATION

Sleipner Project



CO₂ storage mechanisms

- ❖ Hydrodynamic trapping: traps the CO₂ into flow systems for geological periods of time
 - ◆ main concern : CO₂ leakage through imperfect confinement.
- ❖ Solubility trapping: traps the CO₂ in the saline solutions
 - ◆ Main concern: solubility limit and salt out effects
- ❖ Mineral trapping: react with brine and rock matrix to mineralize and immobilize CO₂ (e.g., calcite, dolomite, siderite)
 - ◆ main question: fast enough?
 - ◆ time frame for performance assessment
 - ◆ predictions

CO_2 -Brine-Mineral Interactions

- ❖ For geological sequestration
- ❖ The gas
- ❖ The rock
- ❖ The brine
- ❖ The interactions

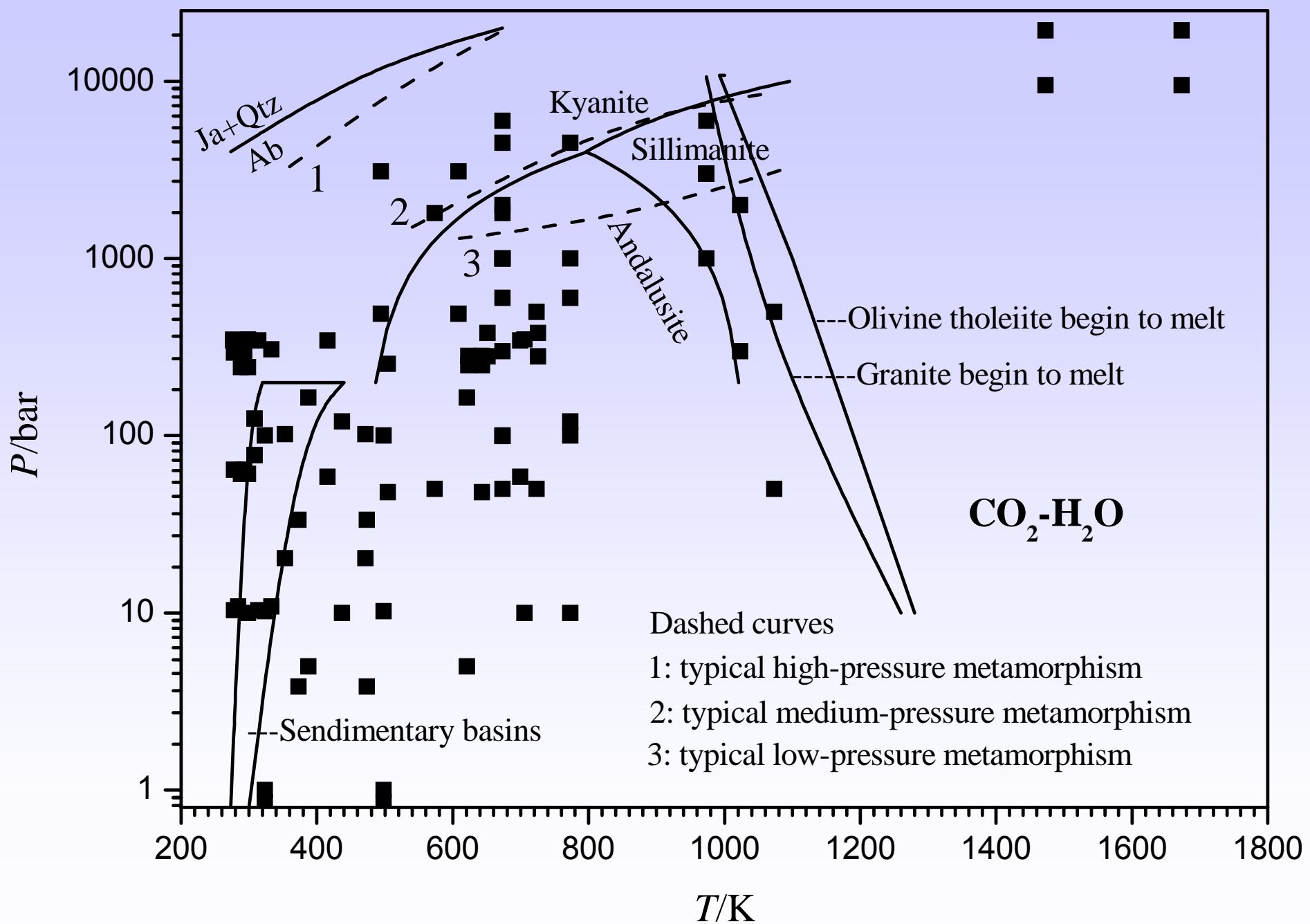
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- ❖ the chemical system (CO_2 - H_2O - SO_2 - NaCl - CaCl_2 - MgCl_2) is extremely complex
 - ❖ temperature (T) ranges from 25 o to 200 °C
 - ❖ pressure (P) up to 500 atmospheres
 - ❖ Salinity up to 300,000 mg/L
 - ❖ The thermodynamic properties of gas-liquid-salt systems are typically described by an Equation of State (EOS), which calculates the quantitative relationships between intensive parameters of systems (e.g., T , P) and extensive parameters (e.g., volume, mass, composition of different phases)
 - ❖ EOS for ideal gas $PV = nRT$

OBJECTIVES

- ❖ **Search the literature and review available experimental data and EOS;**
- ❖ **Recalibrate the current CO₂ solubility models to include recent experimental data; and**
- ❖ **Suggestions for future research**

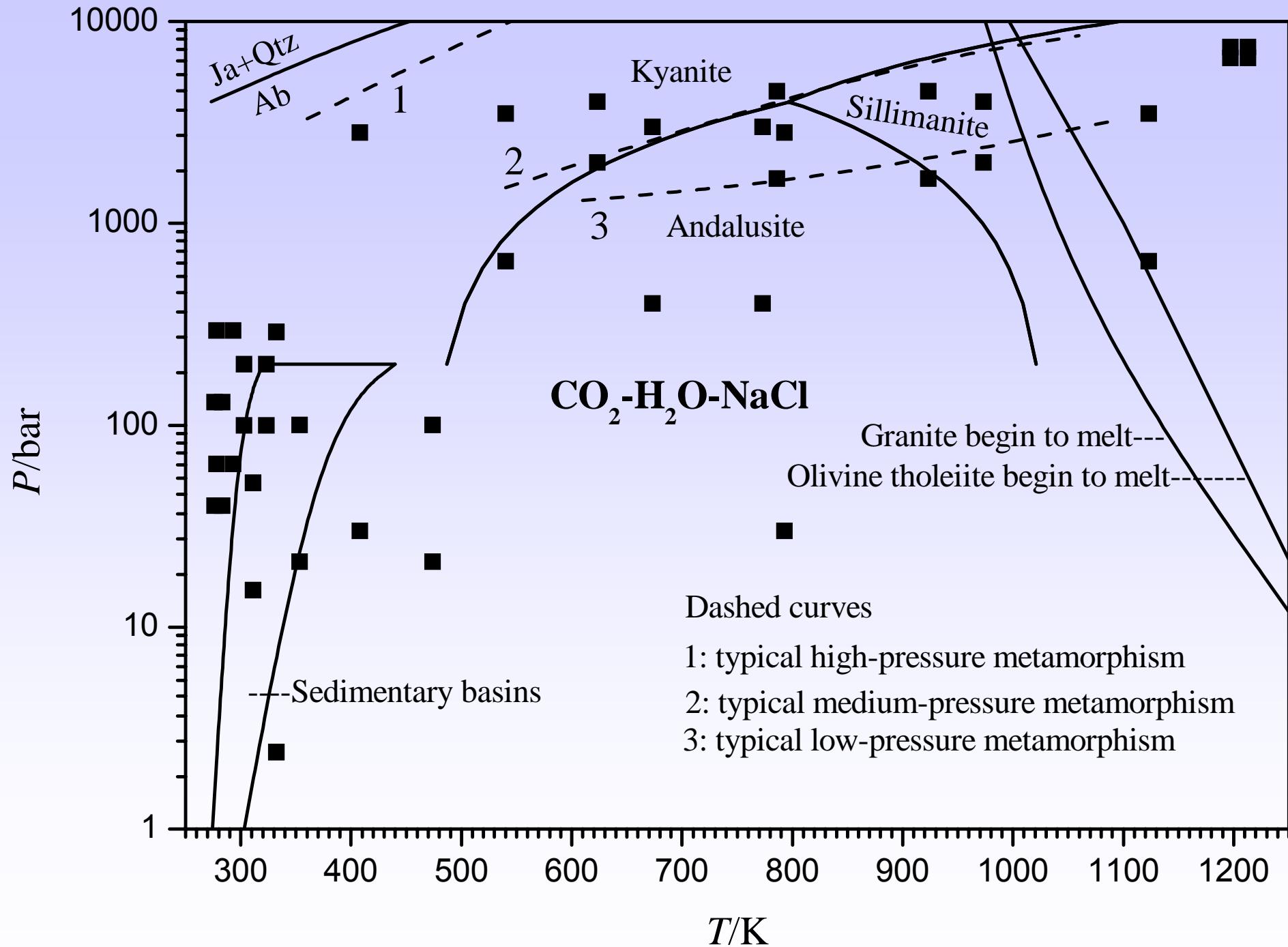
Accomplishments #1

- ❖ A comprehensive survey and evaluation of the experimental $PVTx$ properties and thermodynamic modeling of the systems $\text{CO}_2\text{-H}_2\text{O}$ and $\text{CO}_2\text{-H}_2\text{O-NaCl}$
- ❖ Over 100 references
- ❖ Submitted a manuscript to *Chemical Geology*
- ❖ "*PVTx Properties of the $\text{CO}_2\text{-H}_2\text{O}$ and $\text{CO}_2\text{-H}_2\text{O-NaCl}$ Systems: Assessment of experimental data and thermodynamic models*"



Authors	T/K	P/bar	Concentration	N_d
Ohsumi et al. (1992)	276.15	347.54	$x(\text{CO}_2) \text{ \%} = 0.1798\text{-}0.6294$	5
Teng et al. (1997)	278-293	64.4-294.9	$x(\text{CO}_2) \text{ \%} = 2.50\text{-}3.49$	24
Parkinson & De Nevers (1969)	278.1-313.7	10.342-344.744	$x_{\text{CO}_2} \text{ \% (mol)} = 0.1\text{-}2.2$	28
Hebach et al. (2004)	283.80-333.19	10.9-306.6	$x(\text{CO}_2) = \text{saturated values}$	201
King et al. (1992)	288.15-298.15	60.8-243.2	$x(\text{CO}_2) \text{ \%} = 2.445\text{-}3.070$	27
Hnědkovský et al. (1996)	298.15-705.38	10-350	$m(\text{CO}_2) = 0.155\text{-}0.185$	32
Zhang et al. (2002)	308.15	77.52-124.84	$x(\text{CO}_2) \text{ \%} = 0.3$	16
Patel et al. (1987)	323.15-498.15	0-100	$x(\text{CO}_2) = 0.5\text{-}0.98$	457
Patel & Eubank (1988)	323.15-498.15	0.855-10.237	$x(\text{CO}_2) = 0.02\text{-}0.5$	297
Nighswander et al. (1989)	352.85-471.25	20.4-102.1	$x(\text{CO}_2) \text{ \%} = 0.22\text{-}1.66$	33
Zawisza & Malesińska (1981)	373.15-473.15	3.85-33.5	$y(\text{H}_2\text{O}) = 0.1210\text{-}0.9347$	145
Ellis (1959)	387.15-621.15	5-164	$y(\text{CO}_2) \text{ \%} = 3.90\text{-}6.27\text{-}84.02$	36
Fenghour et al. (1996)	415.36-699.30	58.84-345.77	$x(\text{CO}_2) = 0.0612\text{-}0.7913$	164
Wormald et al. (1986)	437.2-773.2	10-120	$x(\text{CO}_2) = 0.5$	115
Sternér & Bodnar (1991)	494.15-608.15	487-3100	$x(\text{CO}_2) = 0.1234\text{-}0.7473$	84
Franck & Tödheide (1959)	673.15-973.15	1000-6000	$x(\text{CO}_2) = 0.1234\text{-}0.8736$	107
Ellis (1963)	504.15-643.15	47.91-254.43	**	9
Zarikov (1984)	573.15-673.15	50-1800	$x(\text{CO}_2) = 0.2\text{-}0.805$	149
Zhang & Frantz (1992)	519.95-634.45	*	$x(\text{CO}_2) \text{ \%} = 5.5\text{-}16.5$	29
Crovetto & Wood (1992)	622.75-642.70	196.4-281.3	$x(\text{CO}_2) \text{ \%} = 0.48\text{-}0.8745$	72
Crovetto et al. (1990)	651.10-725.51	279.8-380.5	$x(\text{CO}_2) \text{ \%} = 0.130\text{-}1387$	94
Seitz & Blencoe (1999)	673.15	99.4-999.3	$x(\text{CO}_2) = 0.1\text{-}0.9$	95
Gehrig (1980)	673.15-773.15	100-600	$x(\text{CO}_2) = 0.1\text{-}0.9$	198
Shmulovich et al. (1980)	673.15-773.15	1000-4500	$x(\text{CO}_2) = 0.087\text{-}0.6232$	33
Franck & Tödheide (1959)	673.15-1023.15	300-2000	$x(\text{CO}_2) = 0.2\text{-}0.8$	303
Greenwood (1969)	723.15-1073.15	50-500	$x(\text{CO}_2) = 0.1\text{-}0.9$	711
Sternér (1992)	973.15	3000	$x(\text{CO}_2) = 0.375\text{-}0.775$	5

Authors	Precision of T	Precision of P	Precision of composition	Precision of V, Z or d
Ohsumi et al. (1992)				0.0004g·cm ⁻³ (d)
Teng et al. (1997)		0.1 bar		1.9% **
Parkinson & De Nevers (1969)	0.03K			2.4cm ³ ·mol ⁻¹ (average, V_φ)
Hebach et al. (2004)	0.005K	0.5 bar		0.15%
King et al. (1992)			0.3%(H ₂ O-rich)	~0.5%(d)
Hnědkovský et al. (1996)			0.5%(CO ₂ molality)	<1%(V_φ , <625K) 4%(V_φ , ≥625K)
Zhang et al. (2002)	0.03K	0.1 bar		0.01cm ³ (V)
Patel et al. (1987)	1K	0.14 bar		0.05%(d, Z)
Patel & Eubank (1988)	0.01K	0.01%	0.0002-0.0023%	0.05%
Nighswander et al. (1989)	0.5%	0.35 bar	0.02mol%, 0.001g(wt)	0.006g/cm ³ , or 0.8%(d)
Zawisza & Malesińska (1981)	0.005K	0.03%		0.09%(V)
Ellis (1959)			not of high precision	
Fenghour et al. (1996)	0.01K	0.02%		0.08-0.14%(d , average)
Wormald et al. (1986)				
Sterner & Bodnar (1991)	1%(2 σ), 6%V ^{1/2} (σ)	1%(2 σ)	0.0026(x_{CO_2})	6.8%(max, V) 0.8% (average, V)



The experimental $PVTx$ properties of the CO₂-H₂O-NaCl system

Researchers	T/K	P/bar	Concentration	N_d
Song et al. (2004)	276.15-283.15	40-130	$wt(\text{CO}_2)\% = 0\text{-}7.7$ $Sr\% = 3.5\%$	64 ^A
Teng & Yamasaki (1998)	278-293	64.4-294.9	$x(\text{CO}_2)\% = 1.96\text{-}3.27$ $m(\text{NaCl}) = 0.99\text{-}4.99$	24 ^B
Song et al. (2003)	303.15-323.15	100-200	$wt(\text{CO}_2)\% = 1\text{-}4$ Sr=underground brine	99 ^B
Wang et al. (1996)	311	15.24-51.78	$x(\text{CO}_2)\% = 0.39\text{-}1.34$ $Sr\% = 0.25\text{mol/L}$	5
Li et al. (2004)	332.15	2.4-289.3	$c(\text{CO}_2) = 0\text{-}0.958 \times 10^{-3}\text{mol}\cdot\text{cm}^{-3}$ Sr% = Weyburn brine	37 ^C
Nighswander et al. (1989)	353.15-473.65	21.1-100.3	$x(\text{CO}_2)\% = 0.28\text{-}1.54$ $wt(\text{NaCl})\% = 1.0$	34
Gehrig et al. (1986)	408-793	30-2812	$x(\text{CO}_2)\% = 0.18\text{-}84.9$ $Sr\% = 6.0\text{-}20.0$	114
	673-773	400-3000	$x(\text{CO}_2)\% = 0\text{-}100$ $Sr\% = 6.0, 10.0$	279
Krüger & Diamond (2001a)	786.15-923.15	1670-4500	$x(\text{CO}_2)\% = 9.52\text{-}9.84$ $Sr\% = 6.0$	14
Schmidt et al. (1995)	623.15-973.15	2000, 4000	$x(\text{CO}_2)\% = 5$ (relative to H ₂ O) $Sr\% = 40$	14
Krüger & Diamond (2001b)	540-1123	650-3500	$x(\text{CO}_2)\% = 9.69\text{-}21.01$ $x(\text{NaCl})\% = 1.52\text{-}1.74$	Not given
Johnson (1992)	1197.15-1213.15	6600-7458	$x(\text{CO}_2)\% = 0.187\text{-}0.489$ $S_r(\text{NaCl})\% = 14.0\text{-}23.6$	4

Note: A=a specific underground saline water within a Japanese city, B= artificial seawater, C=Weyburn brine, Sr =relative salinity, wt=weight, m=molality, x=mole fraction, c=concentration (mol·cm⁻³)

Precisions of the experimental $PVTx$ properties of the CO₂-H₂O-NaCl system

Researchers	T	P	Concentration	Density/volume
Song et al. (2004)				<1.5%($d\Delta\rho/dW_{\text{CO}_2}$)
Teng & Yamasaki (1998)	0.2K	0.1 bar	1.55%(mol)	1.87%(d)
Song et al. (2003)	0.1K		0.1wt%	0.005%(d)
Wang et al. (1996)	0.2K	0.007bar (0.025%)		$V: 0.001\text{cm}^3$
Li et al. (2004)	0.2K	0.09 bar	$C_{\text{CO}_2}: <2\%$, $W_{\text{H}_2\text{O}}: 0.1\%$	$V: 1\text{cm}^3(0.7\%)$, $d: 10^{-4}\text{gcm}^{-3}$
Nighswander et al. (1989)	0.5%	0.35 bar	0.02%(mol), 0.001g(wt)	0.5cm ³ (V)
Gehrig et al. (1986)	0.5K(~373K), 2K(773K), 5K ($T \geq 673\text{K}$, on phase boundary)	<0.2 bar	0.2mol%	~0.4%(V), <1%(V, high T , $P < 15\text{MPa}$)
Krüger & Diamond (2001a)	3K	20 bar	0.1%(x_{CO_2})	$0.5\text{cm}^3\cdot\text{mol}^{-1}(V)$
Schmidt et al. (1995)	0.5% (~5K when $T > 773\text{K}$)	1%	~1%	~1%

Note: V =molar volume, W =mass fraction, wt =weight, C =concentration in mol·dm⁻³, d =density, $d\Delta\rho/dW_{\text{CO}_2}$ = partial derivative of density difference with respect to the mass fraction of CO₂. Johnson (1992) 5-21K 50-70 bar 0.85-1.22cm³·mol⁻¹(V)

Accomplishment #2. Improved CO₂ solubility model

- ❖ Updated and improved the CO₂ solubility with new experimental data
- ❖ Temperature from 273 to 533 K, pressure from 0 to 2000 bar, and salinity from 0 to 4.5 molality
- ❖ New model with numerical calculation efficiency, suitable to be used in large scale computer models

Accomplishment #2. CO₂ solubility model update

- ❖ Manuscript submitted to *Marine Geochemistry*
- ❖ “An improved model for the calculation of CO₂ solubility in aqueous solutions containing Na⁺, K⁺, Ca²⁺, Mg²⁺, Cl⁻, SO₄²⁻”

Improved CO₂ solubility model

$$\ln m_{CO_2} = \ln y_{CO_2} f_{CO_2} P - m_{CO_2}^{l(0)} / RT - 2l_{CO_2-Na}(m_{Na} + m_K + 2m_{Ca} + 2m_{Mg}) - z_{CO_2-Na-Cl} m_{Cl} (m_{Na} + m_K + m_{Mg} + m_{Ca}) + 0.07 m_{SO4} \quad (1)$$

m molality of CO₂ or salts in the liquid phase

φ fugacity coefficient

γ activity coefficient

μ chemical potential

λ_{CO_2-ion} interaction parameter

$\zeta_{CO_2-cation-anion}$ interaction parameter

Superscripts

v vapor

l liquid

(0) standard state

aq aqueous solution

Non-iterative equation to calculate CO₂ fugacity as a function of ~~temperature and pressure~~

$$f_{CO_2} = c_1 + [c_2 + c_3 T + c_4/T + c_5/(T - 150)]P + [c_6 + c_7 T + c_8/T]P^2 + [c_9 + c_{10}T + c_{11}/T]\ln P + [c_{12} + c_{13}T]/P + c_{14}/T + c_{15}T^2, \quad (2)$$

C – fitted parameter

Experimental CO₂ Solubility data used in regression

Authors	T (K)	P (bar)	N ^a	AAD(%) ^b	Quality ^c
Wiebe and Gaddy (1939)	323-373	25-710	29	1.41	h
Wiebe and Gaddy (1940)	285-313	25-507	42	1.77	h
Markham and Kobe (1941)	273-313	1.01-1.09	3	2.07	h
Harned and Davis (1943)	273-323	1.01-1.14	18	0.94	h
Prutton and Savage (1945)	374-393	23-703	26	3.27	h
Morrison and Billett (1952)	286-348	1.02-1.40	19	3.07	h
Malinin (1959)	473-523	98-490	10	3.24	h
Todheide and Franck (1963)	323-533	200-2000	30	5.16	h
Takenouchi and Kennedy (1964)	383-533	100-1500	76	3.86	h
Takenouchi and Kennedy (1965)	423-523	100-1400	30	3.93	h
Malinin and Savelyeva (1972)	298-348	47.9	11	4.18	m.
Malinin and Kurorskaya (1975)	298-423	47.9	9	4.08	m
Drummond (1981)	303-523	40-126	41	5.12	m
Zawisza and Malesinska (1981)	323-473	1-54	33	5.61	m
Müller et al. (1988)	373-473	3-80	49	2.81	h
Nighswander et al. (1989)	353-471	20-102	33	6.50	m
King et al. (1992)	288-298	60-250	27	1.85	h
Servio and Englezos (2001)	277-283	20-42	9	7.23	m
Anderson (2002)	274-288	1-22	54	1.33	h
Chapoy et al. (2004)	274-351	2-93	27	2.97	h
Valtz et al. (2004)	278-318	5-80	47	4.70	m

CO₂ solubility data not used in the model, but consistent with model calculations

Authors	T (K)	P (bar)	N ^a	AAD(%) ^b	Quality ^c
Kritschewsky et al. (1935)	293-303	5-30	10	4.44	m
Zel'vinskii (1937)	273-373	11-94	80	2.59	m
Bartholomé and Friz (1956)	283-303	1-20	15	1.52	h
Matous et al. (1969)	303-353	10-39	13	2.51	h
Shagiakhmetov and Tarzimanov (1981)	323-373	100-800	9	3.23	m
Gillespie and Wilson (1982)	288-366	7-203	24	4.87	m
Oleinik (1986)	283-343	10-160	23	1.95	h
Briones et al. (1987)	323	68-177	7	2.61	h
D'Souza et al. (1988)	323-348	101-152	4	2.53	h
Dohrn et al. (1993)	323	101-301	3	1.28	h
Teng et al. (1997)	278-293	64-295	24	1.55*	m
Zheng et al. (1997)	278-338	0.49-0.84	10	1.18	h
Dhima (1999)	344	100-1000	7	1.90	h
Bamberger et al. (2000)	323-353	40-141	29	2.62	h
Yang et al. (2000)	298	21-77	9	5.67	m
Rosenbauer et al. (2001)	294	100-600	3	1.76	h
Teng and Yamasaki (2002)	298	75-300	6	1.87	h
Bando et al. (2003)	303-333	100-200	12	2.25	h

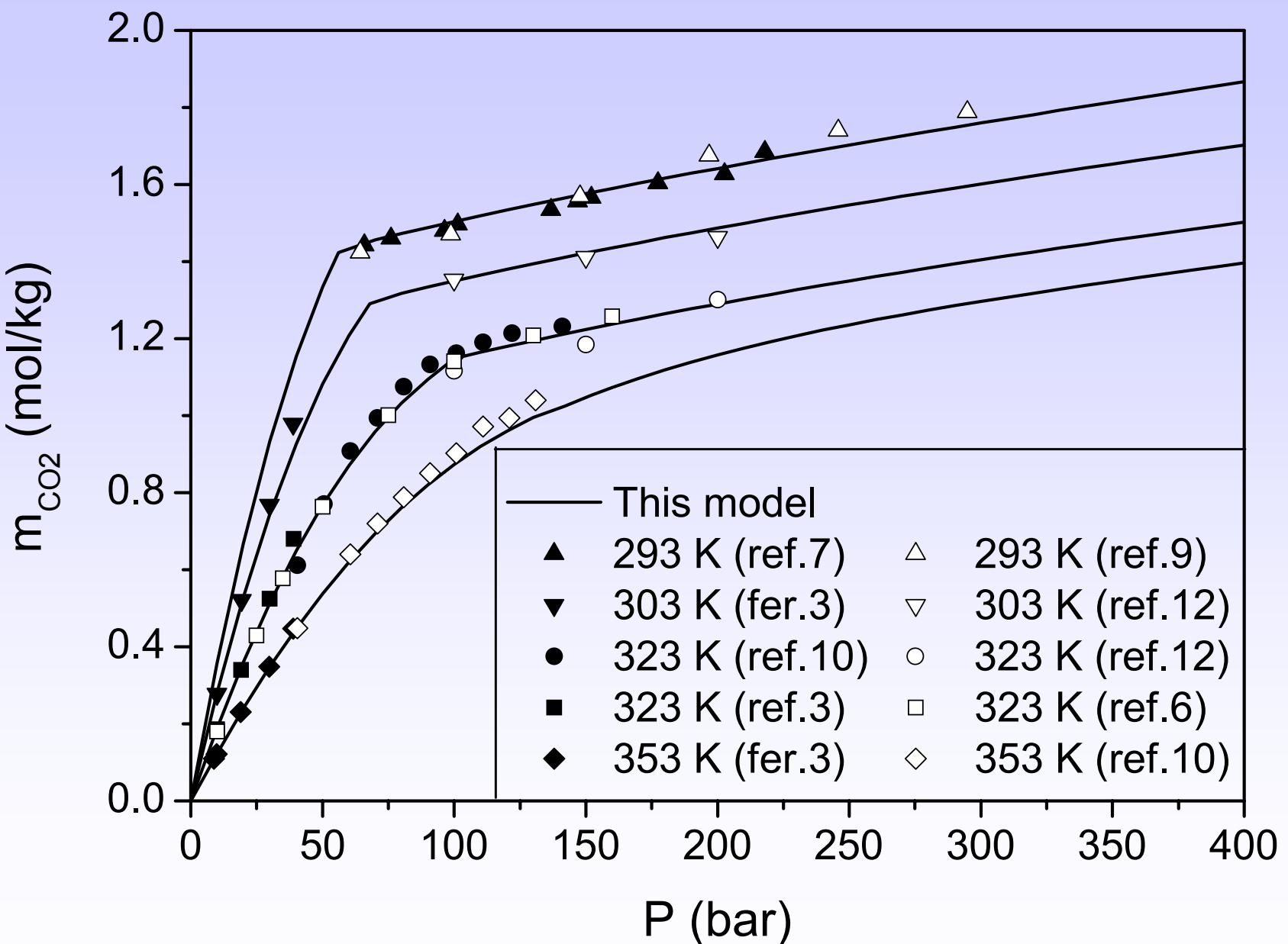


Table 5. CO₂ solubility in 35‰ seawater (The chemical composition of seawater is from Holland (1978)).

P (bar)	T (K)							
	273.15	283.15	293.15	313.15	333.15	353.15	373.15	393.15
1.0	.0655	.0458	.0330	.0200	.0124	.0063	.0000	.0000
5.0	.3159	.2228	.1624	.1030	.0719	.0532	.0396	.0268
10.0	.6042	.4282	.3136	.2011	.1429	.1093	.0873	.0701
25.0		.9478	.7034	.4610	.3346	.2632	.2200	.1914
50.0		1.4647	1.1607	.7911	.5914	.4773	.4098	.3688
75.0		1.4983	1.2729	1.0078	.7792	.6448	.5652	.5190
100.0		1.5309	1.3063	1.0814	.9074	.7720	.6909	.6457
125.0		1.5622	1.3382	1.1140	.9925	.8644	.7908	.7517
150.0		1.5925	1.3688	1.1448	1.0249	.9239	.8686	.8400
175.0		1.6218	1.3983	1.1741	1.0555	.9768	.9257	.9131
200.0			1.4266	1.2020	1.0844	1.0201	.9789	.9709
225.0			1.4541	1.2286	1.1119	1.0566	1.0249	1.0260
250.0			1.4808	1.2542	1.1381	1.0881	1.0652	1.0751
275.0			1.5068	1.2788	1.1631	1.1159	1.1012	1.1192
300.0			1.5322	1.3025	1.1871	1.1410	1.1337	1.1593
325.0			1.5571	1.3255	1.2102	1.1644	1.1635	1.1960
350.0			1.5816	1.3478	1.2324	1.1864	1.1911	1.2299
375.0			1.6058	1.3695	1.2539	1.2076	1.2170	1.2614
400.0			1.6297	1.3908	1.2747	1.2282	1.2415	1.2910
425.0			1.6534	1.4117	1.2950	1.2484	1.2649	1.3190
450.0			1.6770	1.4321	1.3148	1.2684	1.2874	1.3456
475.0			1.7004	1.4523	1.3342	1.2883	1.3092	1.3711
500.0			1.7237	1.4723	1.3532	1.3081	1.3304	1.3955

Table 6. CO₂ solubility in pure water at CO₂ hydrate-liquid water-gas or liquid CO₂ equilibrium

<i>T</i> (K)	<i>P</i> _{eq} (bar) ^a	<i>m</i> _{CO₂} (m)	<i>T</i> (K)	<i>P</i> _{eq} (bar) ^a	<i>m</i> _{CO₂} (m)
270.15	9.729	.7681	281.15	32.78	1.429
270.65	9.915	.7660	281.65	35.22	1.480
271.15	10.11	.7639	282.15	37.94	1.533
271.65	10.30	.7620	282.65	41.01	1.588
272.15	10.49	.7601	283.15	44.54	1.645
272.65	11.52	.8113	283.65	67.04	1.703
273.15	12.20	.8378	284.15	115.9	1.760
273.65	12.92	.8653	284.65	171.5	1.819
274.15	13.68	.8938	285.15	231.7	1.878
274.65	14.50	.9233	285.65	296.3	1.939
275.15	15.37	.9540	286.15	365.2	2.001
275.65	16.31	.9858	286.65	438.3	2.064
276.15	17.31	1.019	287.15	515.8	2.128
276.65	18.37	1.053	287.65	597.7	2.194
277.15	19.52	1.089	288.15	684.2	2.260
277.65	20.75	1.126	288.65	775.7	2.328
278.15	22.08	1.164	289.15	872.3	2.397
278.65	23.51	1.204	289.65	974.6	2.468
279.15	25.06	1.246	290.15	1083.	2.539
279.65	26.74	1.289	290.65	1198.	2.611
280.15	28.57	1.334	291.15	1321.	2.685
280.65	30.58	1.380	291.65	1452.	2.760

Table 7. CO₂ solubility in 35‰ seawater at CO₂ hydrate-seawater-gas or liquid CO₂ equilibrium.

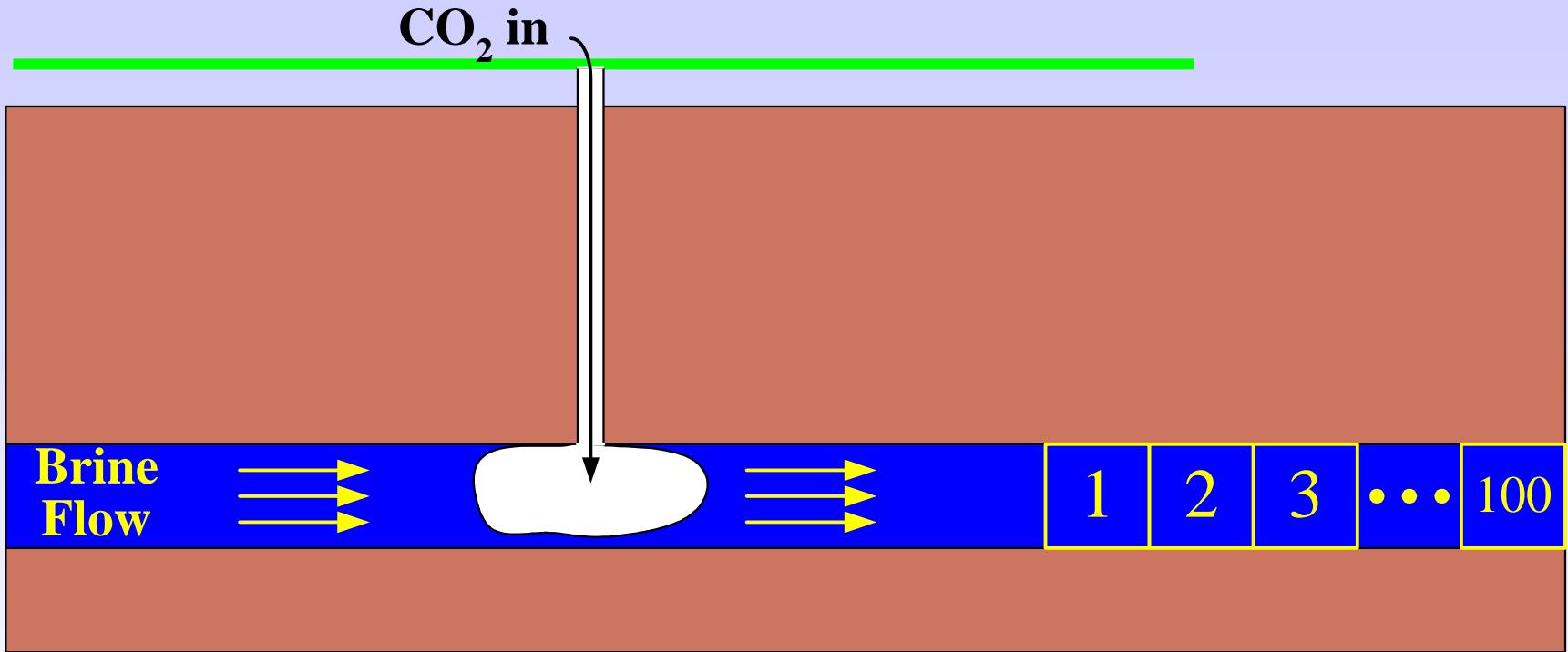
<i>T</i> (K)	<i>P</i> _{eq} (bar)	<i>m</i> _{CO₂} (m)	<i>T</i> (K)	<i>P</i> _{eq} (bar)	<i>m</i> _{CO₂} (m)
270.15	10.04	.6804	279.65	32.22	1.279
270.65	10.62	.7024	280.15	34.64	1.324
271.15	11.25	.7252	280.65	37.34	1.372
271.65	11.91	.7489	281.15	40.40	1.423
272.15	12.62	.7734	281.65	43.93	1.494
272.65	13.37	.7989	282.15	78.24	1.527
273.15	14.18	.8252	282.65	132.4	1.584
273.65	15.03	.8526	283.15	192.4	1.642
274.15	15.95	.8811	283.65	258.2	1.701
274.65	16.93	.9106	284.15	330.0	1.763
275.15	17.98	.9412	284.65	408.3	1.827
275.65	19.11	.9731	285.15	493.7	1.896
276.15	20.33	1.006	285.65	587.0	1.971
276.65	21.64	1.041	286.15	689.8	2.053
277.15	23.05	1.076	286.65	803.9	2.142
277.65	24.58	1.114	287.15	932.3	2.238
278.15	26.24	1.152	287.65	1080.	2.352
278.65	28.05	1.193	288.15	1256.	2.476
279.15	30.04	1.235	288.65	1478.	2.623

^a *P*_{eq} means the pressure of CO₂ hydrate-liquid water-gas or liquid CO₂ phase equilibrium

Synergies

- ❖ Collaboration with NETL in-house research
- ❖ 1D modeling of CO₂-brine-rock interaction
- ❖ Paper in press in *Environmental Geosciences*

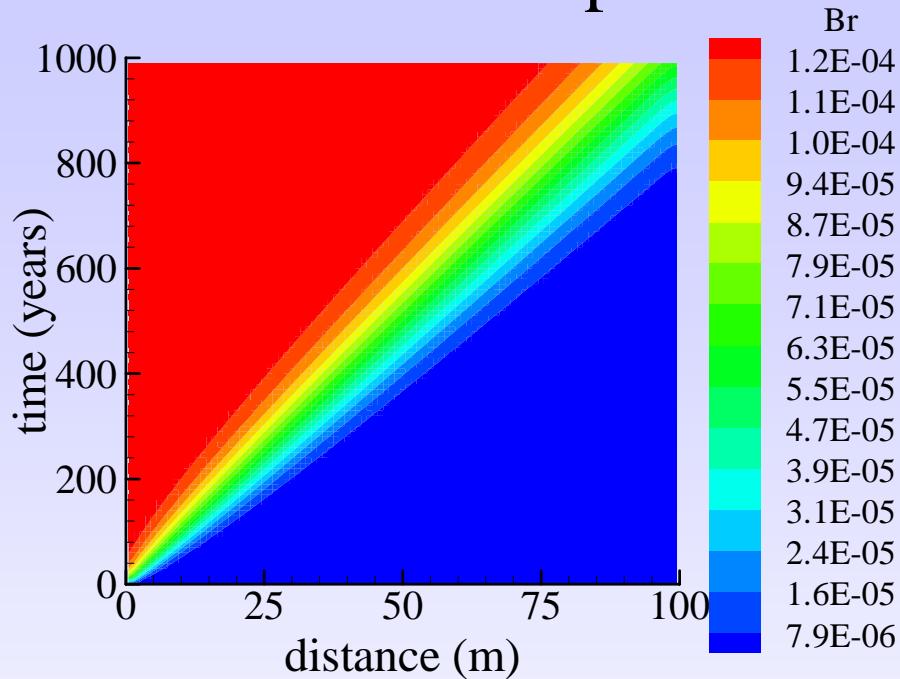
Modeling the fate of injected CO₂



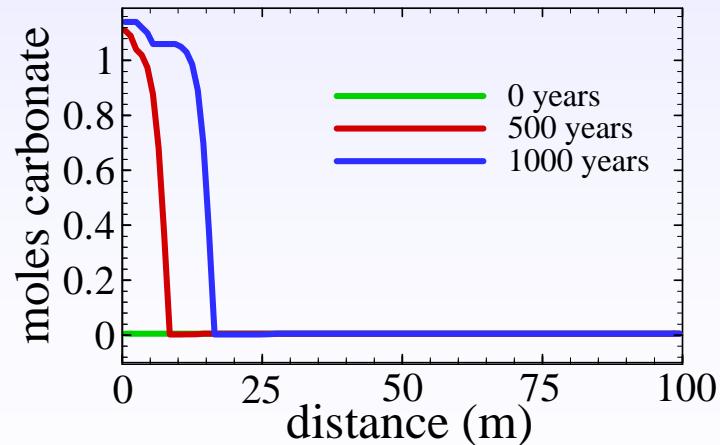
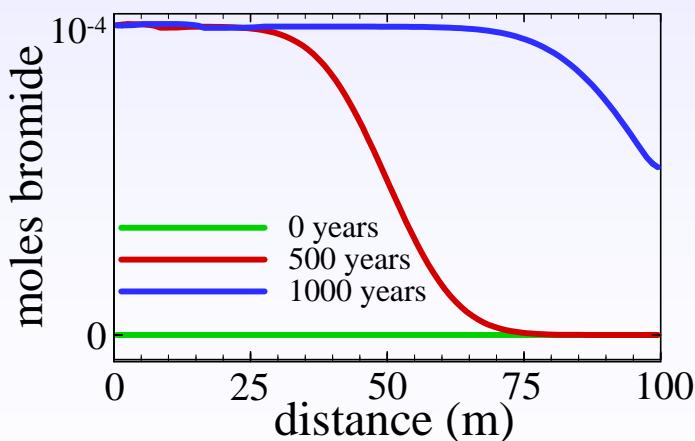
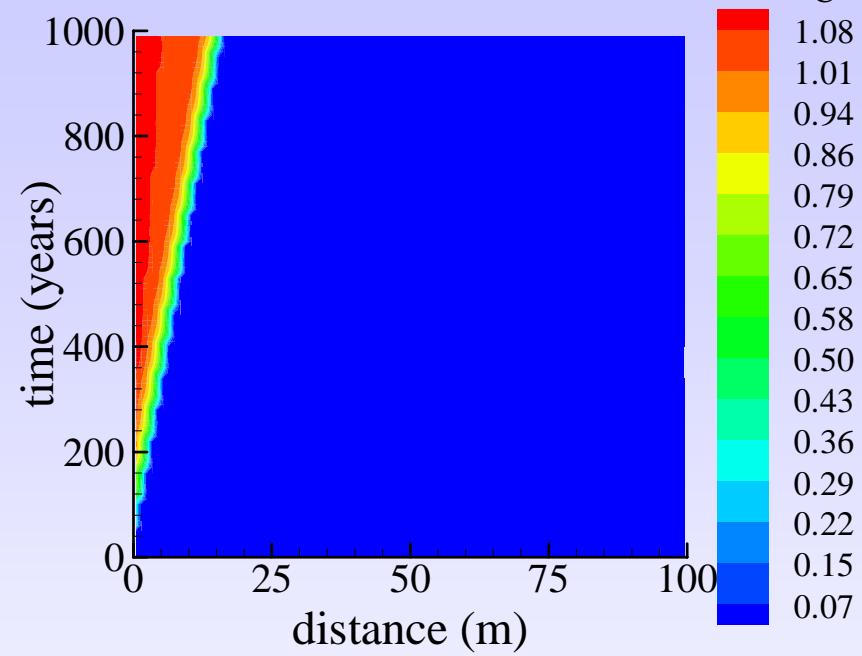
- ❖ Model begins well after CO₂ injection, downstream of the injection site.
- ❖ CO₂ assumed to be dissolved in brine.

Local equilibrium case

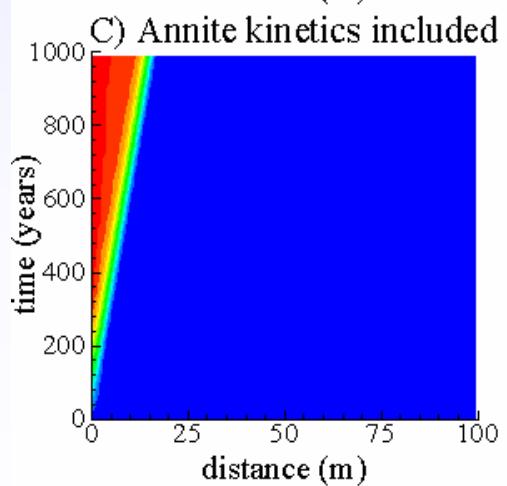
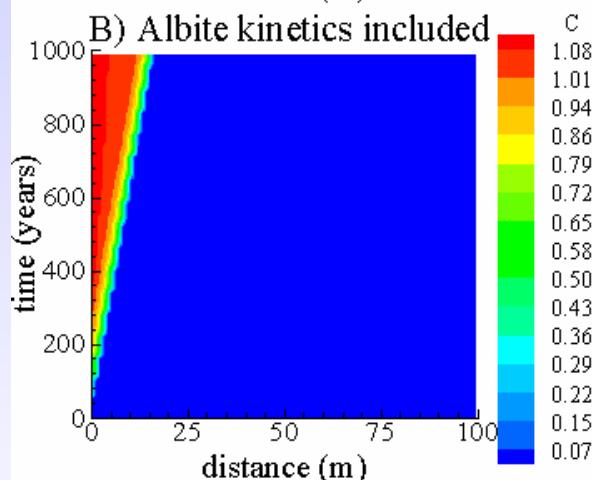
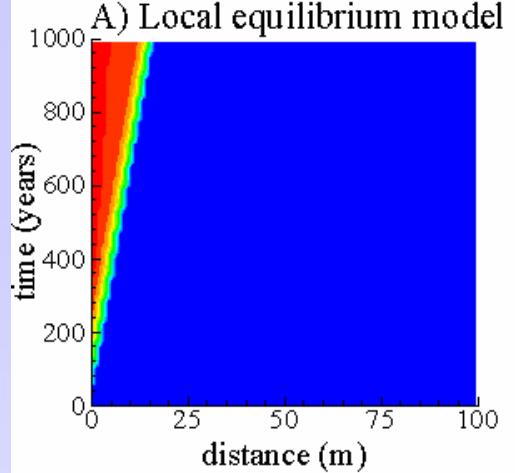
Bromide Transport



Carbonate Transport



With lab dissolution rates



Conclusions

- ❖ Comprehensive review of PTVx data in the $\text{CO}_2\text{-H}_2\text{O}$ and $\text{CO}_2\text{-H}_2\text{O-NaCl}$ system;
 - ◆ A manuscript submitted to Chemical Geology
- ❖ An improved CO_2 solubility model in $\text{CO}_2\text{-H}_2\text{O-SO}_4\text{-NaCl-CaCl}_2\text{-MgCl}_2$ solutions
 - ◆ Updated with new experimental data
 - ◆ More computational efficiency
 - ◆ Accurate prediction of CO_2 solubility
 - ◆ Suitable for geological carbon sequestration (0-260 °C, 0-2000 bars, up to 4.5 molal NaCl equivalent)
- ❖ Identified needs and future work
 - ◆ Experimental data with coexisting phases
 - ◆ Experimental data on volumetric properties
 - ◆ EOS for carbon sequestration must take into account NaCl and CO_2 aqueous dissociation – a major undertaking

A wide-angle photograph of a mountainous landscape at dusk or dawn. In the foreground, a dark lake reflects the surrounding environment. On either side of the lake are large, dark mountain ridges. A small town or cluster of buildings is visible on the far shore of the lake. The sky above is a clear, pale blue, suggesting early morning or late evening light.

Thank you

TASKS TO BE PERFORMED

- ❖ Task 1.0 - Literature Review
- ❖ Evaluation of the suitability of current equation of state for carbon sequestration
- ❖ Task 2.0 – Recalibration of CO₂ solubility model with new experimental data.
- ❖ New experimental data on CO₂ solubility in NaCl and natural brines will be used to recalibrate existing model.
- ❖ Task 3.0 – Calculations of Volumetric Properties in the CO₂-H₂O-NaCl system
- ❖ Volumetric properties for CO₂-H₂O-NaCl system at temperatures suitable for carbon sequestration will be calculated by combining the CO₂ solubility model of Duan and Sun (in press) and Pitzer's volume model for NaCl-H₂O.
- ❖ Task 4.0 – Devise a strategy for long-term research
- ❖ After a thorough literature search, we will learn the need of critical data and make recommendations of future experiments. We will also devise a strategy for further development of EOS suitable for CO₂ sequestration.